Geometries and energy separations of electronic states of GeF2, SnF2, and PbF2 and their positive ions

Dai, D. , Al-Zahrani, M.M. , Balasubramanian, K.

Journal of Physical Chemistry
Vol. 98, Issue.37, 1994

Abstract: Seven singlet and triplet electronic states of GeF2, SnF2, and PbF2 and the 2A1 and 2B1 electronic states of GeF2+, SnF2+, and PbF2+ are investigated. We employed complete active space multiconfiguration self-consistent-field followed by multireference singles + doubles configurations interaction which included up to 1.3 million configurations. Complete bending potential energy surfaces of eight singlet and triplet electronic states of GeF2 are obtained. The ground state of MF2 (M = Ge, Sn, Pb) molecules is the X1A1 state with θc between 92° and 98° while re(M-F) are 1.723, 1.865, and 2.139 A°, respectively. The ground state of MF2+ species is found to be of X2A1 symmetry. The adiabatic ionization potentials are obtained. In addition, spin-orbit effects are included for PbF2 using the relativistic configuration interaction method. Our computed spectroscopic constants of the ground and excited states of GeF2, SnF2, and PbF2 species are in good agreement with both ultraviolet absorption and infrared spectra of these species. The computed bond energies are also in good agreement with the measured values. Several other electronic states are predicted which are yet to be observed.